Spontaneous Peierls dimerization and emergent bond order in one-dimensional dipolar gases

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Abstract. - We investigate the effect of dipolar interactions in one-dimensional systems in connection with the possibility of observing exotic many-body effects with trapped atomic and molecular dipolar gases. By combining analytical and numerical methods, we show how the competition between short- and long-range interactions gives rise to frustrating effects which lead to the stabilization of spontaneously dimerized phases characterized by a bond-ordering. This genuine quantum order is sharply distinguished from Mott and spin-density wave phases, and can be unambiguously probed by measuring non local order parameters via *in-situ* imaging techniques.

Introduction. – Cold atom gases confined in reduced dimensionality represent an ideal system to observe many-body phenomena related to the prominent role played by quantum fluctuations [1, 2]. Recent experimental advances have paved the way to the investigation of quantum magnetism, notable examples being the demonstration of super-exchange interactions in bosonic gases [3], the time-evolution of spin impurities [4, 5], the observation of frustrated classical dynamics [6] and the engineering of Ising Hamiltonians [7].

New opportunities in this direction are now stimulated by the prominent progresses in cooling and controlling ultracold gases of magnetic atoms and polar molecules, which provide tunable platforms where the effect of long-ranged dipolar interactions can play a dominant role in determining the many-body dynamics [8–12]. Such progresses have opened a new door for the investigation of lattice models beyond the conventional Hubbard paradigm, where long-range interactions can compete with local ones on the way to unveil richer many-body physics [13–15]. Much attention has been devoted up to now to extended Bose-Hubbard models, where a new phase of matter, the Haldane insulator (close analog of the Haldane phase in spin-1 chains) has been predicted to occur [16–19]. However, not much is known on other possible magnetic phases for fermionic dipolar gases in optical lattices [15], which present close analogy to the so called extended Hubbard model (EHM) [20–30].

In this Letter we show that one dimensional (1D) Hubbard models with long-range interactions support a non-trivial insulating phase characterized by bond-order [23, 25, 27, 30] [a bond-order density-wave (BOW)] due to the competition between dipolar and on-site interactions. This phase has attracted notable interest in recent years in the context of strongly correlated electron systems. Its existence is now well-established but it has been longly debated in a series of theoretical studies [23–30]. The opportunity of realizing and observing such states of matter may shed new light on a series of issues, from its dynamical properties to its ground state robustness. In order to prove its existence in dipolar Hubbard models, we combined analytical and state-of-the-art numerical methods based on the density-matrix-renormalization-group (DMRG) algorithm [31,32]. Remarkably, the effect of dipolar interaction is evident already in the weak-coupling approach, leading to the prediction of a BOW phase within one-loop order. This is in sharp contrast with standard EHMs - on-site and nearest neighbor interaction only-, where a simple formalism is instead unable to capture its existence [23]. While the detection of the BOW phase is in general challenging

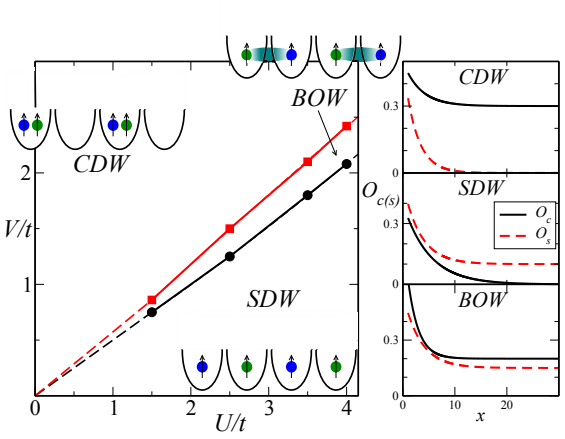

Fig. 1: Panel *a)*: numerical phase diagram for dipolar mixtures described by the Hubbard Hamiltonian in Eq. (2) and corresponding cartoon picture for the different phases. A region with dominant bond-order develops close to the line $U \simeq V\frac{3\zeta(3)}{2}$. Errors in determining phase transition points are smaller than symbol sizes. Panel *b)*: qualitative behavior of different string correlation functions $\mathcal{O}_{c,s}$ in the different phases (CDW, SDW and BOW, from top to bottom): in the BOW phase, both order parameters display long-range-order.

due to the limited extension in parameter space and its lack of density-like order parameters, we show how the recently developed *in situ* imaging techniques [33,34] provide an ideal route toward the unbiased identification of such phases since the BOW phase is uniquely identified by the long-range order of non-local parity correlations [35, 36].

Spin-1/2 dipolar Fermi gas. – Dipolar particles confined in a one dimensional tube can be described by the following microscopic Hamiltonian:

$$H = \int dx \sum_{\sigma=1,2} \left\{ \psi^\dagger_\sigma(x) \left[-\frac{\hbar^2}{2m}\partial_x^2 \right] \psi_\sigma(x) \right\} \quad (1)$$
$$+ \sum_{\sigma,\sigma'} \int dx\, dy \big[\rho_\sigma(x)(\mathcal{V}(x,y) + \mathcal{U}\delta(x,y))\rho_{\sigma'}(y) \big],$$

where m is the particle mass, $\psi^\dagger_\sigma(\psi_\sigma)$ are creation(annihilation) operators of $\sigma = 1, 2$ fermions, and $\rho_\sigma = \psi^\dagger_\sigma\psi_\sigma$. The short-distance contribution of interspecies interactions $\mathcal{U}$ can be tuned by using Feshbach resonances or confinement induced, while the dipolar interaction $\mathcal{V}$ is controlled by means of electric (polar molecules) or magnetic (magnetic atoms) fields [15]. Once confined on a sufficiently deep optical lattice, an effective description in terms of Hubbard Hamiltonian leads to the discrete formulation (see, e.g., [1]):

$$H = -\sum_{\sigma,i} t(c^\dagger_{i,\sigma}c_{\sigma,i+1} + h.c.) + U\sum_i n_{1,i}n_{2,i}$$
$$+ \sum_{i<j}\sum_{\sigma,\sigma'} V_{\sigma,\sigma'}(|i-j|)n_{\sigma,i}n_{\sigma',j}, \quad (2)$$

where the on-site interaction U is now given by a combination of local and dipolar potential, and the last term describes long-range dipolar interactions, $V_{\sigma,\sigma'}(|i-j|) = V/(|i-j|)^3$, which we consider purely repulsive from here on. In the equal mass, equal interaction case, the system inherits a global $SU(2)$ symmetry, which is preserved by the long-range tail, and is reduced to $U(1)$ for general parameter choices. From here on, we will focus on the former case and consider a balanced half-filled chain, $N_1 = N_2 = N/2 = L/2$, where N_σ is the number of particles in the spin state σ and L the system size. Like in the case of the EHM, the phase diagram of Eq. (2) is determined by the competition between local and non-local interactions. Before searching for specific BOW instabilities, we illustrate the competing mechanism in the atomic limit $t = 0$, as such competition will then lead to spin-frustration at the origin of bond-order itself.

For dominant U interactions, the system ground state is a spin density wave (SDW). On the other hand, a dominant dipolar interaction will minimize the energy by imposing double occupancies every second site, thus stabilizing a fully gapped charge density wave (CDW). These two ground states, illustrated in the insets of Fig. 1, become energetically degenerate along the line $U_c^{(cl)} = 3\zeta(3)V/2$ (ζ is the Riemann zeta function), which determines a phase transition between SDW and CDW. Deeply in the quantum regime $t \simeq V \simeq U$, however, quantum fluctuations may enhance the emergent frustration close to the classical transition line and lead to a different critical scenario. For the EHM, where only nearest-neighbor interactions are considered, it was argued by Nakamura [23] that an additional phase with dominant charge bond-order instability occurs between the SDW and the CDW phases. This phase is characterized by a spontaneous spin-Peierls dimerization, manifest in a charge polarization on alternating bonds and by the formation of spin dimers on the bonds, and constitutes a notable example of dimerization in strongly correlated systems due to frustration. A 2D analog of this phase has been recently discussed for spinless dipolar fermions in layers [37].

The existence and extent of the BOW phase in the EHM have been intensively debated mainly because *i)* the instability is not captured by one-loop g-ology calculations based on bosonization (while more refined methods recently provided analytical evidence of it [25, 29]), and *ii)* numerical results were not consistent due to the small extent in parameter space of such a phase, and to the difficulty of providing accurate location of the critical line [23, 26, 27, 30]. In the following, combining analytical and numerical methods, we show that dipolar systems support spontaneous spin-Peierls dimerization, and that the corresponding BOW phase occupies a larger region in parameter space with respect to the EHM. First of all, we show that one-loop g-ology is sufficient to establish the existence of bond-order in the weak-coupling regime. Then, the existence and extent of the BOW phase are bench-

marked with DMRG simulations.

Low-energy field theory. – We now present a qualitative study of Eq. (2) within the bosonization framework [38]. As a first step, we express the fermionic lattice operators in terms of continuum chiral fields $\psi^\dagger_{R/L}(x)$:

$$c^\dagger_{j,\sigma} = \sqrt{a}[\psi^\dagger_{R,\sigma}(x)e^{ik_F x} + \psi^\dagger_{L,\sigma}(x)e^{-ik_F x}], \qquad (3)$$

with $x = ja$, a the lattice spacing and $k_F = \pi N/(2La)$ the Fermi momentum. We then apply the standard bosonization mapping introducing density and phase fluctuation fields $\varphi_\sigma, \vartheta_\sigma$ for the two species in order to map the original fermionic problem onto a bosonic one:

$$\psi_{R,\sigma} = \frac{\eta_{R,\sigma}}{\sqrt{2\pi a}} e^{-i[\varphi_\sigma - \vartheta_\sigma]}, \quad \psi_{L,\sigma} = \frac{\eta_{L,\sigma}}{\sqrt{2\pi a}} e^{i[\varphi_\sigma + \vartheta_\sigma]} \qquad (4)$$

where $\eta_{r,\sigma}$ are the so-called Klein factors. We proceed by first bosonizing independently the single species Hamiltonians, and then consider the coupling between them. This allows us to partially keep track of the long-ranged dipolar interactions by using known results on single channel Luttinger liquids (LL) with dipolar interactions [39–42]. The single species Hamiltonian can then be bosonized as follows:

$$\begin{aligned} H_\sigma &= \frac{\hbar v}{2}\int dx \left[\frac{(\partial_x\varphi_\sigma)^2}{K} + K(\partial_x\vartheta_\sigma)^2\right] \\ &+ g\int dx \cos[\sqrt{4\pi}\varphi_\sigma] \end{aligned} \qquad (5)$$

where v is the sound velocity, and the Luttinger parameter K is well approximated as $K = (1 + 1.46n * V/t)^{-1/2}$ [42]. An additional mass term due to the lattice is also present. While these results strictly hold in the continuum, they well capture the quantitative dependence of K with respect to interaction and filling fraction even in lattice models [43]. We can now proceed and treat local and non-local interspecies interactions as a perturbation on the top of $H_1 + H_2$. After introducing density and spin collective fields:

$$\varphi_{c/s} = \frac{\varphi_1 \pm \varphi_2}{\sqrt{2}}, \quad \vartheta_{c/s} = \frac{\vartheta_1 \pm \vartheta_2}{\sqrt{2}}, \qquad (6)$$

the Hamiltonian can be decoupled into a density and spin sector, $H = H_c + H_s$, where the physics in each sector is described by a sine-Gordon model:

$$\begin{aligned} H_{c/s} &= \frac{\hbar v_{c/s}}{2}\int dx \left[\frac{(\partial_x\varphi_{c/s})^2}{K_{c/s}} + K_{c/s}(\partial_x\vartheta_{c/s})^2\right] \\ &+ g_{c/s}\int dx \cos[\sqrt{8\pi}\varphi_{c/s}]. \end{aligned} \qquad (7)$$

Notice that terms coupling density and spin degrees of freedom are also present; in the following we will neglect their effects, which are supposed to be small away from the regime $V, U \ll t$ due to their large scaling dimension. Within first order g-ology, the parameters of the effective Hamiltonian can be estimated as follows: first, we compute the effect of the interspecies interactions on the quadratic part of the Hamiltonian by approximating the interspecies dipolar interactions up to next-nearest-neighbor. The effective Luttinger parameters then read:

$$K_{c/s} = \sqrt{K\left(\frac{1}{K} \pm \frac{U + 9V/4}{4\pi t}\right)^{-1}}. \qquad (8)$$

The coefficient g_s of the mass term in the spin sector is then fixed by imposing SU(2) spin symmetry in H_s. This leads to a Berezinskij-Kosterlitz-Thouless (BKT) transition [38] which takes place at $K_s = 1$, that is, in the weak-coupling limit, $V_c^{(BKT)} \simeq U/2.34$. In the repulsive regime $U, V > 0$, the density sector is instead expected to be always gapped since $K_c < 1$, except on the line $g_c = 0$ which identifies a Gaussian transition (at strong coupling, this line can be unstable toward $4k_F$ mass terms when $K_c < 1/4$). Since the coefficient of the mass term is $g_c \propto (U + 7V/4)$, the Gaussian transition can be identified at $V_c^{(G)} = U/1.75$.

The phase diagram can be subsequently mapped out by considering the dominant orders as in the case of the EHM [23]. For $V \lesssim U/2.34$, the system is in a SDW phase, with a gapless spin sector and dominant correlations of the form $\langle(n_{i,\uparrow} - n_{i,\downarrow})(n_{i+x,\uparrow} - n_{i+x,\downarrow})\rangle$. On the other hand, a (mass) density-wave is formed above the critical value $V > V_c^{(G)}$, where the dominant correlations are of the form $\langle(n_{i,\uparrow} + n_{i,\downarrow})(n_{i+x,\uparrow} + n_{i+x,\downarrow})\rangle$. In the intermediate regime $V_c^{(BKT)} < V < V_c^{(G)}$, neither SDW nor CDW order are stable, and the system exhibits a BOW, characterized by both a finite spin and density gap, and a dominant order described by the parameter

$$\langle B_i\rangle = \langle\frac{1}{2}\sum_\sigma \left(c^\dagger_{i,\sigma}c_{i+1,\sigma} + c^\dagger_{i+1,\sigma}c_{i,\sigma}\right)\rangle. \qquad (9)$$

This indicates that dimers are spontaneously formed on nearest-neighbor bonds, a phenomenon usually called as spontaneous spin-Peierls dimerization.

As such, we conclude that, even within one-loop g-ology, the low-energy theory already predicts a finite region of parameter space where bond order is stable. This is due to the effects of the long-range dipolar tails, which consistently affect the Luttinger parameter of the single species Hamiltonians, and lead to different conditions for the BKT and Gaussian transition. However, the treatment is supposed to work only in the weak-coupling regime, and the provided estimate on the Gaussian line does not indeed capture the entire dipolar interactions. In order to confirm this qualitative view, we provide in the following a numerical analysis of Eq. (2).

Numerical results. – The accurate determination of the phase diagram of the system is a very challenging task. As far as the simpler EHM is concerned, despite the great effort put in its numerical study over the last decade, few results have shown good agreement with each other [24,26,

27, 30]. Mindful of the difficulties in the determination of the phase diagram for such a system, we carefully checked our methods and codes on the EHM with both periodic (PBC) and open boundary conditions (OBC); discarded weights of the order 10^{-8} allow us to estimate the phase transitions within 1% with the most recent and accurate results [30].

We calculate several physical quantities to determine as accurately as possible the two phase boundaries of Eq. (2), keeping in the DMRG simulation terms up to $|j-i|=5$ in the off-site dipolar interaction part. We verified for small system sizes that the inclusion of longer range terms does not affect significantly the quantities of interest.

CDW-BOW transition. Starting in the CDW phase, as the dipolar interaction strength is decreased the system enters in a BOW phase. As a first probe of the transition, we calculate the density gap

$$\Delta_c = \lim_{L\to\infty} \left[E(N+2,0) + E(N-2,0) - 2E(N,0)\right]/2 \tag{10}$$

where $E(N,S_z)$ is the ground state energy of $N=L$ particles with total magnetization $S_z=(N_\uparrow - N_\downarrow)/2$. Due to the competition between long range and on-site interactions the gap has to take a minimum value at the transition point. To locate the phase boundary as precisely as possible we also calculate the BOW order parameter defined as

$$\langle B\rangle = lim_{L\to\infty} |\langle B_{L/2} - B_{L/2+1}\rangle|, \tag{11}$$

where B_i is the operator in Eq. (9). $\langle B\rangle$ is the amplitude of the oscillation of the BOW operator at the center of the chain, defined in such a way that Friedel oscillations are weaker [44]: a non-vanishing value of $\langle B\rangle$ will be a clear signature of the BOW phase.

A further signature of the phase transition is given by the LL parameter K_c. For a periodic chain it can be extracted from the (density) static structure factor

$$S_c(q) = \frac{1}{L}\sum_{k,l} e^{iq(k-l)} \left(\langle n_k n_l\rangle - \langle n_k\rangle\langle n_l\rangle\right) \tag{12}$$

with $q=2\pi/L$. Within LL theory $K_c = \lim_{q\to 0} \pi S_c(q)/q$ is finite only on the phase transition line for a continuous transition (while is always zero instead for first order transitions). Since we are dealing with a finite size system we expect to see a sharp peak at the transition line varying the dipolar interaction.

In order to get the correct values in the thermodynamic limit for the quantities described above, a careful finite size scaling analysis must be carried out. The density gap Δ_c is extrapolated fitting the data with a fourth-order polynomial in $1/L$. For the BOW order parameter $\langle B\rangle$ we assume that in the centre of the chain the amplitude of Friedel oscillations is proportional to $1/L^{K_c}$ [44] to extrapolate its thermodynamic value.

We run several DMRG simulations for different dipolar interaction strengths V and system sizes (till $L=128$) with OBC. We keep up to $m=1256$ states and perform 6 sweeps to calculate the density gap and the BOW order parameter. In this way the truncation error, i.e., the weight discarded in the renormalization procedure, is at most of order 10^{-8}, while the error on the energies is approximately 10^{-8}. To calculate the static structure factor (12), we instead use PBC on smaller systems ($L=16,24,32,40,48$), but the same number of states and sweeps as for OBC.

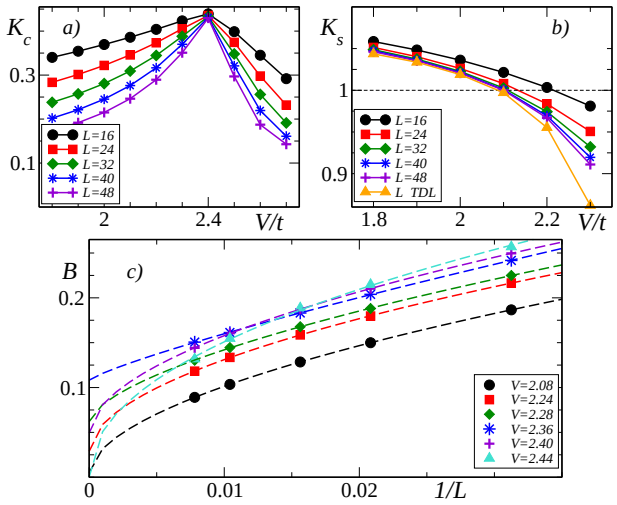

Fig. 2: Panels *a)* and *b)*: Luttinger parameters K_c and K_s respectively, as functions of V for different L; orange triangles are the values of K_s in the thermodynamic limit (TDL). Panel *c)*: BOW order parameter $\langle B\rangle$ for various V. Straight lines are guides for the eye, whereas dashed lines fit the numerical data using the appropriate scaling laws.

The results for the CDW-BOW transition are reported – for $U=4t$ – in panels *a)* and *c)* of Fig. 2 and panel *a)* of Fig. 3. In particular one sees that K_c develops a peak (sharper as the system size increases) when $V/t\simeq 2.4$, the BOW order parameter $\langle B\rangle$ vanishes as $V/t=2.44$ while it is still finite for $V/t=2.4$ and the density gap has a minimum also at $V/t=2.4$. Thus we can infer that the transition between the CDW and the BOW phases occurs for $V/t\simeq 2.4$.

SDW-BOW transition. As the strength of the dipolar interaction is further decreased, Peierls dimerization is destroyed and the system enters in a SDW with a uniform distribution of the density and no gap in the spin sector. The BKT nature of this transition makes its location challenging when evaluating the spin gap

$$\Delta_s = \lim_{L\to\infty} \left[E(N,1) + E(N,0)\right] \tag{13}$$

since it is exponentially small close to the transition line [38]. A valid alternative is provided by the spin-static structure factor

$$S_s(q) = \frac{1}{L}\sum_{k,l} e^{iq(k-l)} \left(\langle s^z_k s^z_l\rangle - \langle s^z_k\rangle\langle s^z_l\rangle\right). \tag{14}$$

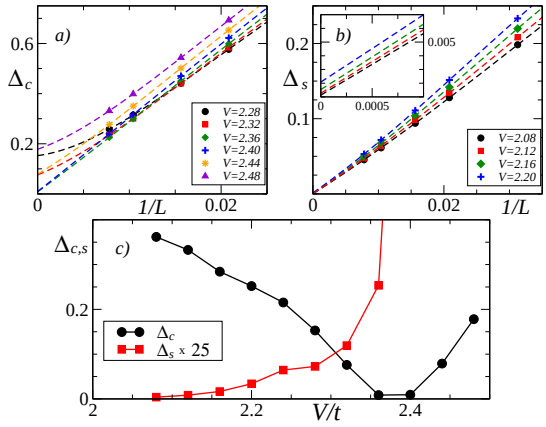

Fig. 3: Panels *a)* and *b)*: charge Δ_c and spin gaps Δ_s respectively, for various V; a magnification is illustrated in the inset in panel *b)*. Panel *c)*: density and spin ($\times 25$) gaps in the thermodynamic limit for various V. Straight lines are guides for the eye, whereas dashed lines fit the numerical data using the appropriate scaling laws.

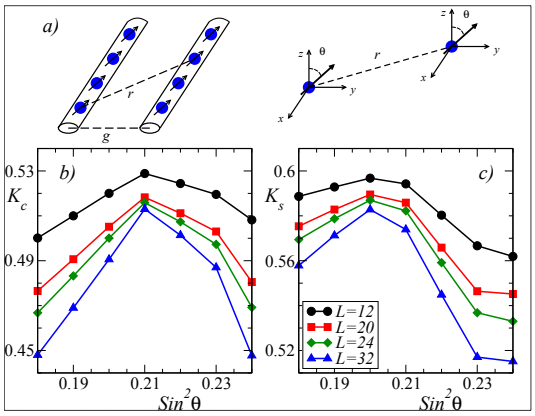

Fig. 4: Panel *a)*: schematic cartoon of ladder configuration. Panels *b)*-*c)*: K_c and K_s as a function of the angle θ for different system sizes for the case $d_1 = d_2 = 1.5$ and $g = 1.0$

Indeed LL theory predicts that $K_s = \lim_{q\to 0} \pi S_s(q)/q$ is zero in the spin gapped phase and $K_s = 1$ in the gapless one. Logarithmic corrections prevent K_s to reach the latter value even for long chains. Nonetheless, such corrections have been shown to vanish in the frustrated $J - J'$ model when the system forms dimers [45]. The same is true for the EHM [27], since the BOW-SDW transition should have the same nature, and thus also for our model. In the BOW phase $K_s = 0$ near the transition only for very large systems. Following [27] we estimate the transition point when, at fixed U, K_s crosses 1 from above as V is increased. The thermodynamic limit of the spin gap Δ_s is obtained, as for the density gap, fitting the data with a fourth-order polynomial in $1/L$, reproducing the spinon band structure near the band edges.

The results of the DMRG simulations are reported in panel *b)* of Fig. 2 and panel *b)* of Fig. 3. First of all one can see that K_s crosses 1 for $V/t \leq 2.1$ and an accurate finite size scaling allows us to locate the transition point for $V/t = 2.089$. This result for the phase transition point is also confirmed by both $\langle B \rangle$ and the spin gap, that have a small, but still finite value (precisely $\langle B \rangle = 5.1 \times 10^{-3}$ and $\Delta_s = 1.6 \times 10^{-4}$) at $V/t = 2.08$.

Dipolar 2-leg ladder. – We have also analyzed a different configuration, which requires single species fermionic dipoles. The gas is confined in two parallel tubes at a distance g and the dipoles (the external electric or magnetic field) form an angle θ with the plane of the wires as sketched in Fig. 4 *a)*. The system can be modelled by the Hamiltonian

$$H_l = -\sum_{a=1,2,i} t\left[c^\dagger_{i,a}c_{i+1,a} + h.c.\right] + \sum_{a=1,2,i} d^2 \frac{n_{i,a}n_{j,a}}{|i-j|^3} + \sum_{a,b=1,2}\sum_{i,j} d^2 \frac{1-3\sin^2\theta}{r^3} n_{i,a}n_{j,b} \quad (15)$$

where $a, b = 1, 2$ are the tube indices, t the hopping parameter and d the dipole momentum, and r denotes the distance between particles in different tubes. We performed DMRG simulations with PBC for system sizes $L = 12, 20, 24, 32$ to calculate the LL parameters K_c and K_s for several values of the angle θ. The results are reported in panels *b)* and *c)* of Fig.4; by applying an analysis similar to the one presented above, we conclude that, whilst a BOW phase may indeed exist for intermediate tilting angles, its extent, indicated by the maxima of the Luttinger parameters, would be much smaller than that for the single tube Fermi mixture.

Experimental regimes and probes. – Polar molecules and magnetic atoms offer strong versatility in tuning interactions. In the latter case, the ratio V/U can be independently tuned by means of Feshbach resonances, which have been already reported for bosonic ^{52}Cr [14] and ^{167}Er [12] isotopes. In case of molecular gases stable under two-body recombination, accurate estimates of on-site interactions will be required. An alternative approach can employ Feshbach molecules of strongly magnetic atoms such as Er or Dy, effectively increasing by a factor ~ 8 the strength of the dipole-dipole interactions [42].

The existence of the BOW phase can be indirectly probed spectroscopically as follows: first, the density gap is estimated by means of lattice modulation spectroscopy, indicating the onset of the Gaussian transition. Subsequently, the spin gap is estimated by means of RF spectroscopy. The BOW phase can be located in the intermediate region between the two transition point, as illustrated

in Fig. 3c. A more solid, direct probe of the exotic nature of the insulating state is the long-range nature of the parity order parameters:

$$\mathcal{O}_s(x) = \langle \prod_{j=\ell}^{\ell+x} e^{i\pi S^z_j} \rangle, \quad \mathcal{O}_c(x) = \langle \prod_{j=\ell}^{\ell+x} e^{i\pi n_j)} \rangle, \qquad (16)$$

which are well-defined order parameters for general Hubbard models [35]. As discussed in Ref. [35,36] and as illustrated in Fig. 1 *b)-d)*, such correlation functions properly distinguish the CDW, SDW and BOW phases. In particular only the latter phase has long-range order in both $\mathcal{O}_s$ and $\mathcal{O}_c$. Although measuring parity order parameters is a difficult task, recently $\mathcal{O}_c$ has been measured for cold atoms with short range interaction loaded in an optical lattice by *in situ* imaging of the many-body wave function via atom fluorescence [34].

Conclusions. – In summary, we have provided a detailed study of how dipolar fermionic mixtures support exotic insulating states with dominant bond-order. We have underpinned the corresponding Hubbard phase diagram by combining numerical and analytical techniques. Remarkably, differently from the standard EHM, we find that the BOW phase can be found already at the level of one-loop g-ology. This is due to the long-range nature of the interaction which enhances the frustration of the system. We also briefly discuss how single species loaded in ladder geometries do not represent a favorable platform to investigate bond-ordered phases.

Experimentally the non-trivial correlations embodied in the bond-density-wave phase can be faithfully captured by spin and density string order parameter by means of *in situ* imaging. This makes cold atoms in optical lattices an ideal setup for the investigation and demonstration of bond-order instabilities in strongly correlated systems.

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